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Machine Learning and Statistical Tools for Decoding Supramolecular Assemblies

Lalit Kumar[1] and Dr. Ashish Narain Dubey[2]
Research Scholar, Department of Chemistry[1]
Research Guide, Department of Chemistry[2]
NIILM University, Kaithal, Haryana, India

Abstract: *Supramolecular chemistry, the study of non-covalent interactions between molecules, is essential for understanding biological systems, material design, and drug delivery mechanisms. However, the complexity and variability of these interactions necessitate robust analytical tools. This paper explores the integration of machine learning (ML) and statistical methods to decode supramolecular assemblies, providing insights into binding dynamics, thermodynamic properties, and structural organization. The study highlights key ML techniques, such as regression models, clustering, and neural networks, alongside statistical tools for multivariate analysis and thermodynamic modeling. By combining computational efficiency with analytical rigor, these approaches enable a deeper understanding of supramolecular systems and facilitate advancements in chemistry and material sciences.*

Keywords: Data-Driven Modeling, Predictive Analytics, Molecular Interactions